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Accurate and Efficient Atomistic-to-Continuum Coupling Methods

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Atomistic-to-continuum coupling methods are a class of computational multiscale schemes that combine the accuracy of atomistic models of crystal defects with the efficiency of continuum elasticity. They are increasingly being utilized in materials science to study the fundamental mechanisms of material failure such as crack propagation and plasticity where crystal defects are coupled to other effects through long-range elastic fields.
In the construction of atomistic-to-continuum coupling methods, various approximation errors are committed. In this project, a rigorous numerical analysis approach that classifies and quantifies these various errors has been given that has enabled the optimization of the atomistic core size, blending, continuum mesh, and far field approximation for accuracy and computational cost. These results have given confidence in the simulation results, as well as enabled the optimization of the numerical methods for accuracy and computational cost.
An analysis and corroborating benchmark computational experiments have been given for blended energy-based and force-based a/c methods that show that these methods are the most efficient and accurate a/c methods for the computation of the deformation of crystals with defects.

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Jean-Luc Cambier, Program Manager

Accurate and Efficient Atomistic-to-Continuum Coupling Methods

Final Report
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Mitchell Luskin
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1. Introduction

Atomistic-to-continuum coupling methods are a class of computational multiscale schemes that combine the accuracy of atomistic models of crystal defects with the efficiency of continuum elasticity. They are increasingly being utilized in materials science to study the fundamental mechanisms of material failure such as crack propagation and plasticity where crystal defects are coupled to other effects through long-range elastic fields.

In the construction of atomistic-to-continuum coupling methods, various approximation errors are committed. In this project, a rigorous numerical analysis approach that classifies and quantifies these various errors has been given that has enabled the optimization of the atomistic core size, blending, continuum mesh, and far field approximation for accuracy and computational cost. These results have given confidence in the simulation results, as well as enabled the optimization of the numerical methods for accuracy and computational cost. We reviewed and extended the numerical analysis foundations of atomistic-to-continuum coupling methods developed in this project in [5].

An analysis and corroborating benchmark computational experiments have been given for blended energy-based and force-based a/c methods that show that these methods are the most efficient and accurate a/c methods for the computation of the deformation of crystals with defects. Extensions of these methods and their analysis has been initiated to compute finite temperature equilibrium, dynamics, and transition rates.

2. Blended energy-based atomistic-to-continuum methods

We formulated an energy-based atomistic-to-continuum coupling method based on blending the quasicontinuum method for the simulation of crystal defects [6]. We utilized theoretical results from to derive optimal choices of approximation parameters (blending function and finite element grid) for microcrack and di-vacancy test problems and confirm our analytical predictions in numerical tests.

In our blended energy-based atomistic-to-continuum method (BQCE), the ghost forces are not eliminated but are controlled in terms of an additional approximation parameter (the blending

width). BQCE applies to a wide range of problems for which no ghost force free energy-based methods are known; these problems include three-dimensional crystals with general many-body interactions as well as multi-lattices. This makes it an attractive method for such challenging and physically important problems.

The implementation of BQCE requires the choice of two approximation parameters: a *blending function* β and a finite-element mesh $\mathbb{T}$ which is used to compute the continuum contribution to the energy. We gave optimal choices of β and $\mathbb{T}$ to minimize global error norms for the problem of a point defect in a 2D crystal based on theoretical results.

We demonstrate the validity of these results in computational test problems in which we simulated a microcrack and a di-vacancy.

3. Blended force-based atomistic-to-continuum methods

We also formulated an atomistic-to-continuum coupling method based on blending atomistic and continuum forces [3, 4]. Our precise choice of blending mechanism is informed by theoretical predictions. We have published a range of numerical experiments studying the accuracy of the scheme, focusing in particular on its stability. These experiments confirmed and extended the theoretical predictions, and demonstrated a superior accuracy of B-QCF over energy-based blending schemes.

We presented numerical experiments to validate and extend our theoretical results for blended force-based atomistic-to-continuum methods. In particular, we studied (i) whether stability of the B-QCF method in 2D can be systematically improved with increasing the blending width, (ii) whether a relatively narrow blending, as suggested by the theory, is enough in practice, and (iii) whether using the quintic spline (that has the regularity assumed in the theory) has advantages over the cubic spline. Our numerical benchmarks demonstrated that the B-QCF scheme is a practical a/c coupling mechanism with performance (accuracy versus computational cost) superior to energy-based blending schemes.

4. Finite temperature atomistic-to-continuum methods

While the recent development of the so-called "hot-QC method" enables dynamic simulations at finite temperature, the times accessible to these simulations remain limited to the sub-microsecond time scale due to the small time step required for stability of the numerical integration. To address this limitation, we developed a novel finite-temperature QC method that can treat much longer time scales by coupling the hot-QC method with hyperdynamics — a method for accelerating time in MD simulations [1, 2, 10]. We refer to the new approach as "hyper-QC". As in the original hyperdynamics method, hyper-QC is targeted at dynamical systems that exhibit a separation of time scales between short atomic vibration periods and long waiting times in metastable states. Acceleration is achieved by modifying the hot-QC potential energy to reduce the energy barriers between metastable states in a manner that ensures that the characteristic dynamics of the system are preserved.

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[2] Woo Kyun Kim, Mitchell Luskin, Danny Perez, Ellad Tadmor, and Art Voter. Hyper-QC: An accelerated finite-temperature quasicontinuum method using hyperdynamics. *Journal of the Mechanics and Physics of Solids*, 63:94–112, 2014.

[3] Xingjie Helen Li, Mitchell Luskin, and Christoph Ortner. Positive-definiteness of the blended force-based quasicontinuum method. *SIAM J. Multiscale Modeling & Simulation*, 10:1023–1045, 2012. arXiv:1112.2528v1.

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[8] D. Olson, P. Bochev, M. Luskin, and A. Shapeev. An optimization-based atomistic-to-continuum coupling method. *SIAM. J. Numer. Anal.*, 52:2183–2204, 2014.

[9] D. Olson, P. Bochev, M. Luskin, and A. Shapeev. Analysis of an optimization-based atomistic-to-continuum coupling method for point defects. *Mathematical Modelling and Numerical Analysis*, to appear. arXiv:1411.4027.

[10] Gideon Simpson and Mitchell Luskin. Numerical analysis of parallel replica dynamics. *Mathematical Modelling and Numerical Analysis*, 47:1287–1314, 2013. arXiv:1204.0819.

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Mitchell Luskin

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Abstract

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5) Woo Kyun Kim, M. Luskin, Danny Perez, Ellad Tadmor, and Art Voter. Hyper-QC: An accelerated finite-temperature quasicontinuum method using hyperdynamics. Journal of the Mechanics and Physics of Solids, 63:94–112, 2014.

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8) D. Olson, P. Bochev, M. Luskin, and A. Shapeev. An optimization-based atomistic-to-continuum coupling method. SIAM. J. Numer. Anal., 52: 2183–-2204, 2014.

9) D. Olson, P. Bochev, A. Shapeev, and M. Luskin. Analysis of an optimization-based atomistic-to-continuum coupling method for point defects. Mathematical Modelling and Numerical Analysis, to appear.

10) Andrew Binder, Mitchell Luskin, Danny Perez, and Arthur F. Voter Analysis of transition state theory rates upon spatial coarse-graining. SIAM J. Multiscale Modeling & Simulation, to appear.

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